Total dielectronic recombination rate coefficient for Ar-like tungsten

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(Received 20 August 1997)

Ab initio calculations of the total dielectronic recombination (DR) rate coefficient for Ar-like tungsten (W^{56+}) are performed using the relativistic HULLAC code package based on the parametric potential method. The high efficiency of HULLAC compared to other codes enables us to perform extensive DR calculations for highly complex atomic systems such as Ar-like tungsten. The present work provides a general procedure for computing the DR rate coefficients for multielectron high-Z ions. This procedure is applicable to DR computations for other Ar-like ions, as well as for ions in neighboring isoelectronic sequences. In the present work level-by-level calculations are performed for evaluating the contributions to DR through all the relevant K-like autoionizing inner-shell excited configuration complexes: $3p^5 4ln'l'$ ($4 \leqslant n' \leqslant 17$), $3s3p^6 4ln'l'$ ($4 \leqslant n' \leqslant 12$), $3p^5 3dn'l'$ ($8 \leqslant n' \leqslant 18$), $3s3p^6 3dn'l'$ ($7 \leqslant n' \leqslant 18$), $2p^5 3s^2 3p^6 3dn'l'$ ($3 \leqslant n' \leqslant 8$), $2s2p^6 3s^2 3p^6 3dn'l'$ ($3 \leqslant n' \leqslant 5$), and $3p^5 5l5l'$. In addition, extrapolation methods are developed to calculate the contributions of even higher n' complexes along each complex series. In the case of $3p^5 3dn'l'$, the usual complex-by-complex extrapolation method based on the n'^{-3} scaling law is found to be inaccurate; thus, a more detailed level-by-level procedure is discussed. All calculations are carried out assuming no electron collisions occur after the initial electron capture. Although the dominant DR contributions come from $3p^5 4ln'l'$ and $3p^5 3dn'l'$, the contributions of the other complex series cannot be neglected. A comparison between the present results and the Burgess-Merts (BM) approximation shows that at low electron temperatures the BM approximation greatly underestimates the DR rate coefficients, whereas at high electron temperatures this approximation is fairly good. [S1050-2947(98)10604-2]

PACS number(s): 34.80.Kw

I. INTRODUCTION

Tungsten is one of the main materials used for plasma facing divertor plates in thermonuclear fusion devices as in the ASDEX upgrade [1]. Tungsten is believed to be favorable for divertors in the next generation of nuclear fusion devices as well [2]. For divertor plasma modeling and radiative plasma cooling studies, accurate atomic data for highly ionized tungsten is necessary, especially data on recombination processes that are a major source of radiation losses. Dielectronic recombination (DR) is the most important recombination process in highly ionized low-density plasmas. Therefore, a precise knowledge of DR processes is necessary for ionization balance modeling.

Due to the complexity of the multielectron ions and to the very large number of inner-shell excited levels that must be included in the calculations, only a few *ab initio* computations were published for DR of ions with 13 electrons or more. Recently calculations of the DR rate coefficients for Ni-like Gd [3] and Ta [4] have been published. Two other works [5,6] were then performed systematically along the Ni I isoelectronic sequence for ten ions. In the Ar I isoelectronic sequence there is a work by Fournier *et al.* [7] that includes the calculation of the total DR rate coefficient for Mo^{24+}. For Ar-like tungsten (W^{56+}) we have calculated in a previous work [8] partial rate coefficients for DR through a few low-lying configuration complexes of the K-like ion.

In the present work extensive *ab initio* level-by-level calculations of all the main DR contributions for Ar-like W are performed, including the following K-like autoionizing inner-shell excited configuration complexes: $3p^5 4ln'l'$ ($4 \leqslant n' \leqslant 17$), $3s3p^6 4ln'l'$ ($4 \leqslant n' \leqslant 12$), $3p^5 3dn'l'$ ($8 \leqslant n' \leqslant 18$), $3s3p^6 3dn'l'$ ($7 \leqslant n' \leqslant 18$), $2p^5 3s^2 3p^6 3dn'l'$ ($3 \leqslant n' \leqslant 8$), $2s2p^6 3s^2 3p^6 3dn'l'$ ($3 \leqslant n' \leqslant 5$), and $3p^5 5l5l'$. Electron inelastic collisions after the initial capture are neglected.

For the low-lying inner-shell excited configuration complexes the effect of radiative *decays* to *autoionizing* levels possibly followed by radiative *cascades* (DAC) is calculated and is found to be of a few percent or even less. Based on the discussion in Refs. [5,6] we will assume here that this is true for higher complexes as well. Consequently, in the present DR calculations for the high-lying complexes DAC processes were neglected.

Furthermore, extrapolation methods are used to evaluate the contributions of the very-high-n' complexes. In order to choose the appropriate extrapolation method a detailed investigation of the behavior of the DR rate coefficients as a function of n' is carried out for each complex series. For the complex series $3p^5 4ln'l'$, $3s3p^6 4ln'l'$, $3s3p^6 3dn'l'$, and $2p^5 3s^2 3p^6 3dn'l'$ the ordinary complex-by-complex extrapolation method is used, whereas for the $3p^5 3dn'l'$ series a more elaborate level-by-level extrapolation procedure is chosen. In addition, the l' dependence of the DR rate coefficients of the various configurations considered in this work is checked and an explanation for the cases where significant contributions of high-l' configurations are found is suggested.

The total contribution of each of the various complex series considered in this work to the total DR rate coefficient is presented and analyzed. Finally, the detailed level-by-level computations are compared with the results obtained by using the approximate Burgess-Merts semiempirical formula.

II. THEORETICAL METHOD

The dielectronic recombination process of Ar-like ions can best be illustrated by using the case of the $3p^5 3dnl$ inner-shell excited configuration complexes. The first step in this process is an *electron capture* by the Ar-like ion in the ground state ($3p^6$) into an inner-shell excited level of the K-like ion lying above the first ionization limit. This step, which is reversible by autoionization, can be schematically written as follows:

$$[\text{Mg core}]3p^6 + e^- \leftrightarrow [\text{Mg core}]3p^5 3dnl, \tag{1}$$

where e^- is the free interacting electron and [Mg core] stands for the full $1s^2 2s^2 2p^6 3s^2$ electronic inner subshells. The second step in the process is a *radiative stabilizing* transition into a final level of the K-like ion lying below the ionization limit. It can take place in one of the following ways:

$$[\text{Mg core}]3p^5 3dnl \rightarrow [\text{Mg core}]3p^6 nl + h\nu, \tag{2a}$$

$$[\text{Mg core}]3p^5 3dnl \rightarrow [\text{Mg core}]3p^5 3dn'l' + h\nu. \tag{2b}$$

Here $h\nu$ represents an emitted photon. In the radiative decay process (2a) the final level $3p^6 nl$ lies below the ionization limit for any value of n and l. In contrast, in the process (2b) the level $3p^5 3dn'l'$ can either be below the ionization limit or above it depending on the values of n' and l'. In the latter case either autoionization occurs or stabilization is reached after one or more additional radiative transitions (cascades):

$$[\text{Mg core}]3p^5 3dn'l' \rightarrow [\text{Mg core}]3p^5 3dn''l'' + h\nu, \tag{2c}$$

$$[\text{Mg core}]3p^5 3dn'l' \rightarrow [\text{Mg core}]3p^6 n'l' + h\nu, \tag{2d}$$

where $3p^5 3dn''l''$ is a final level lying below the ionization limit. If the $3p^5 3dnl$ level lies high enough above the first ionization limit autoionization to the $3p^5 3d$ excited configuration of the Ar-like ion is also possible:

$$[\text{Mg core}]3p^5 3dnl \rightarrow [\text{Mg core}]3p^5 3d + e^-. \tag{3}$$

The rate coefficient β_{kd}^C for the capture of a free electron by an Ar-like ion in its ground level k [process (1)] to form a K-like ion in an inner-shell excited level d above the ionization limit can be evaluated using the principle of detailed balance. Assuming a Maxwellian velocity distribution corresponding to an electron temperature T_e one obtains for the capture rate coefficient the following relation (see, for example, Ref. [9]):

$$\beta_{kd}^C = 1.656\times 10^{-22}(kT_e)^{-3/2}\frac{g_d}{g_k}A_{dk}^a \exp\left(\frac{-E_{dk}}{kT_e}\right), \tag{4}$$

where E_{dk} is the energy difference between the level d and the first ionization limit k. E_{dk} and kT_e are expressed in eV. A_{dk}^a is the coefficient for autoionization from level d to level k expressed in s^{-1}. g_d and g_k are the statistical weights of the levels d and k, respectively. β_{kd}^C is expressed in $cm^3\,s^{-1}$.

Assuming the ion does not undergo inelastic collisions with electrons after the capture of the free electron, the inner-shell excited K-like ion in level d can either autoionize back to form an Ar-like ion in a level k or k' or decay radiatively. This decay can be to a level i below the ionization limit (i.e., effective recombination) or to a level d' above the ionization limit. From the level d' the K-like ion can further either autoionize or decay radiatively. Considering all the possible processes, the *branching ratio* for (effective) *dielectronic recombination* through the level d is given by [6]

$$B^D(d) = \frac{\sum_i A_{di} + \sum_{d'>k} A_{dd'}B^D(d')}{\sum_{k'} A_{dk'}^a + \sum_i A_{di} + \sum_{d'} A_{dd'}}. \tag{5}$$

Here ΣA_{di} and $\Sigma A_{dd'}$ are the sums of the Einstein coefficients for spontaneous emission from level d to levels i and d', respectively. $\Sigma A_{dk'}^a$ is the sum of the autoionization coefficients from level d to levels k' of the Ar-like ion. $B^D(d')$ is the branching ratio for dielectronic recombination via d', defined by a recursive expression analogous to Eq. (5).

For the lower complexes (in each complex series) all the radiative decays from level d to other lower autoionizing levels d' possibly followed by radiative cascades were included in the calculations. Following Refs. [5,6] these processes are referred to as DAC (*decays* to *autoionizing* levels possibly followed by radiative *cascades*). The DAC transitions were found to have an effect of a few percent at the most, as was already noticed and explained in Ref. [5]. Hence, neglecting DAC for higher complexes would lead to an even smaller error in the total DR rate coefficient. Disregarding DAC consists of neglecting all radiative decays to autoionizing levels. This leads to the following approximation for the DR branching ratio:

$$B^D(d) \approx \frac{\sum_i A_{di}}{\sum_{k'} A_{dk'}^a + \sum_i A_{di}}. \tag{6}$$

The rate coefficient for *effective* DR, i.e., for process (1) plus process (2a) or plus processes (2b) and (2c) or (2d), from the initial ground level k of the Ar-like ion through a given intermediate inner-shell excited level d to any final nonautoionizing level i of the K-like ion is given by

$$\alpha_{kd}^D = \beta_{kd}^C B(d). \tag{7}$$

The total rate coefficient for DR from the initial level k is obtained by summing over all the relevant d levels:

$$\alpha_k^D = \sum_d \alpha_{kd}^D. \tag{8}$$

The level-by-level calculations are performed for each series of configuration complexes up to a specific value of the principal quantum number n', denoted by n_s, whose meaning is explained in the following.

In order to evaluate the contributions of the higher complexes ($n' > n_s$) in each complex series extrapolation meth-

ods are used. For the complex series $3p^5 4ln'l'$, $3s3p^6 4ln'l'$, $3s3p^6 3dn'l'$, and $2p^5 3s^2 3p^6 3dn'l'$ the DR rate coefficients start to scale like n'^{-3} from relatively low n' values and the usual complex-by-complex extrapolation procedure can be used. According to this method, first proposed by Hahn [10], the total DR rate coefficient for a given complex series is

$$\sum_{n'=n_0}^{\infty} \alpha^D(n') = \sum_{n'=n_0}^{n_s} \alpha^D(n') + \sum_{n'=n_s+1}^{\infty} \left(\frac{n'}{n_s}\right)^{-3} \alpha^D(n_s). \tag{9}$$

$\alpha^D(n')$ is the total rate coefficient of a configuration complex defined by n'. n_0 represents the lowest value of n' for which the corresponding complex contains levels above the first ionization limit. n_s is the lowest n' value from which $\alpha^D(n')$ starts to scale accurately enough as n'^{-3}.

In contrast to all the other cases, for the complex series $3p^5 3dn'l'$ the n'^{-3} behavior begins at *very-high-n'* values. Therefore, a more elaborate method based on level-by-level extrapolation is needed in order to avoid calculations for too-high-n' values. This method was also proposed by Hahn [10] and was used in the calculations of DR rate coefficients of ions isoelectronic to lighter elements (see, for example, Ref. [11]). The method relies on the fact that for intermediate n' values, even if the DR rate coefficients do not yet scale as n'^{-3}, the radiative and autoionization coefficients for individual levels already have a smooth and known dependence on n'. It is necessary to distinguish here between two different kinds of rate coefficients. The rate coefficients $\beta^C_{kd}, A^a_{dk'}$ and the radiative coefficients A^{hi}_{di} for transitions that do involve the $n'l'$ excited electron (with high principal quantum number n') scale as n'^{-3}. In contrast, the radiative rate coefficients A^{lo}_{di} for transitions which involve the $3d$ excited electron (with low principal quantum number) are constant as a function of n'. Consequently, the total rate coefficient for DR through the whole complex series can be written in this case as follows (neglecting DAC processes):

$$\begin{aligned}\sum_{n'=n_0}^{\infty} \alpha^D(n') &= \sum_{n'=n_0}^{n_s} \alpha^D(n') + \sum_{d \in 3p^5 3dn_s l'} \beta^C_{kd} \sum_{n'=n_s+1}^{\infty} \left(\frac{n'}{n_s}\right)^{-3} \\ &\times \frac{\sum_i A^{lo}_{di} + \left(\frac{n'}{n_s}\right)^{-3} \sum_{i'} A^{hi}_{di'}}{\left(\frac{n'}{n_s}\right)^{-3} \sum_{k'} A^a_{dk'} + \sum_i A^{lo}_{di} + \left(\frac{n'}{n_s}\right)^{-3} \sum_{i'} A^{hi}_{di'}}.\end{aligned} \tag{10}$$

Here, n_s is the lowest n' value from which the radiative and autoionization coefficients start to show a regular behavior (as n'^{-3} or constant) and d is any level of the $3p^5 3dn_s l'$ complex.

All the detailed autoionizing and nonautoionizing level energies and radiative decay coefficients were computed using the *fully* relativistic multiconfiguration RELAC code [12]. The autoionization coefficients were calculated in the semirelativistic distorted-wave approximation using the factorization-interpolation model implemented in the HULLAC code package [13]. This method has been applied in many cases and successfully tested by comparison to more time-consuming methods for calculating autoionization rates [13,14]. In the case of capture from F- to Ne-like ions, for instance, the agreement was found to be better than 5% [13].

Configuration mixing within each complex is taken into account for the lowest autoionizing complexes in each complex series, where it can be significant. For high complexes the mixing is much less important and is neglected.

III. RESULTS AND DISCUSSION

We present here the results of the detailed level-by-level calculations of the rate coefficients for dielectronic recombination through the following K-like tungsten autoionizing inner-shell excited configuration complexes: $3p^5 4ln'l'$, $3s3p^6 4ln'l'$, $3p^5 3dn'l'$, $3s3p^6 3dn'l'$, $2p^5 3s^2 3p^6 3dn'l'$, $2s2p^6 3s^2 3p^6 3dn'l'$, and $3p^5 5l5l'$.

A. DR through the $3p^5 4ln'l'$ complexes

The $3p^5 4ln'l'$ complex series gives the largest contribution to the total DR rate coefficient at low electron temperatures ($kT_e < 100$ eV) and at high electron temperatures ($kT_e > 1$ keV). At $kT_e = E_I$ (5.34 keV) it contributes about 50% of the total DR rate coefficient (see Sec. III H). In this series the lowest complex $3p^5 4l4l'$ is already partially above the ionization limit. All the levels of the complexes $3p^5 4ln'l'$ with $n' \geqslant 5$ are above the ionization limit.

The radiative decay processes that are included in the computations in this case are

$$3p^5 4ln'l' \rightarrow 3p^6 4l + h\nu, \tag{11}$$

as well as alternative decays to the higher K-like configurations: (a) $3p^6 n'l'$, (b) $3p^5 3d4l$, (c) $3p^5 3dn'l'$ ($n' \leqslant 13$), and (d) $3p^5 4ln''l''$ ($n'=4$, $n''=4$) or ($n'=5$, $n''=4,5$). All of the lower levels considered in the computations are below the ionization limit [for this reason $n' \leqslant 13$ in process (c)], except for the two lowest complexes of the series ($3p^5 4l4l'$ and $3p^5 4l5l'$). For these complexes DAC processes of the form (d) are also included. In fact, the DAC processes are found to have negligible effect on the rate coefficient of the $3p^5 4l4l'$ complex. For the $3p^5 4l5l'$ complex DAC processes increase the rate coefficient by 7% at electron temperatures higher than 2 keV.

The energetically possible autoionization processes included in the calculations are

$$3p^5 4ln'l' \rightarrow 3p^6 + e^-, \tag{12}$$

as well as autoionization to the higher Ar-like configurations: (a) $3p^5 3d$ and (b) $3p^5 4l''$ ($n' \geqslant 8$).

Autoionizing inner-shell excited configurations with $0 \leqslant l' \leqslant 8$ are included in the DR calculations. Figure 1 presents for instance the results of the DR rate coefficients for the $3p^5 3d15l$ and $3p^5 4d15l$ configurations. As can be seen from the lower curve, the contributions of configurations with $l > 8$ are expected to be negligible for $3p^5 4d15l$. This

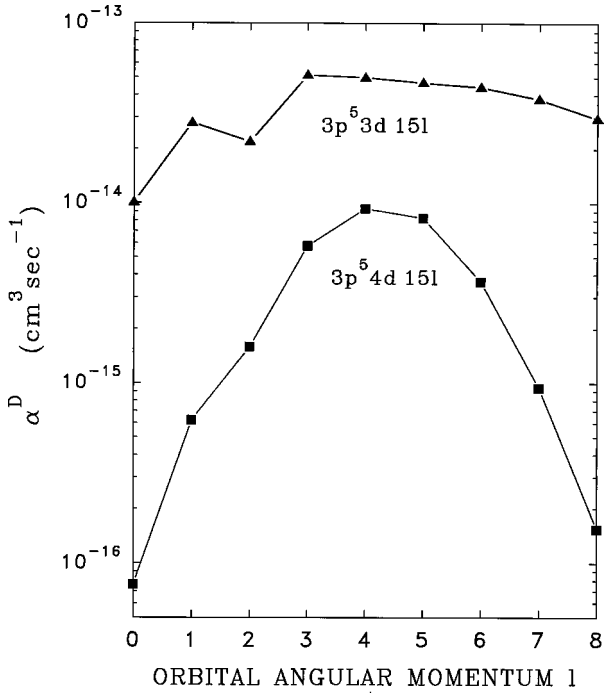

FIG. 1. Partial rate coefficients for DR through the configurations $3p^5 3d 15l$ (triangles) and $3p^5 4d 15l$ (squares) as a function of the orbital angular momentum quantum number l, at an electron temperature of 7 keV. The lines between the calculated values are plotted just to guide the eye.

conclusion is found to be also valid for the other $3p^5 4l 15l$ configurations. The reason for this trend is the steep decrease of the autoionization rate coefficients as l increases, as shown in Fig. 2.

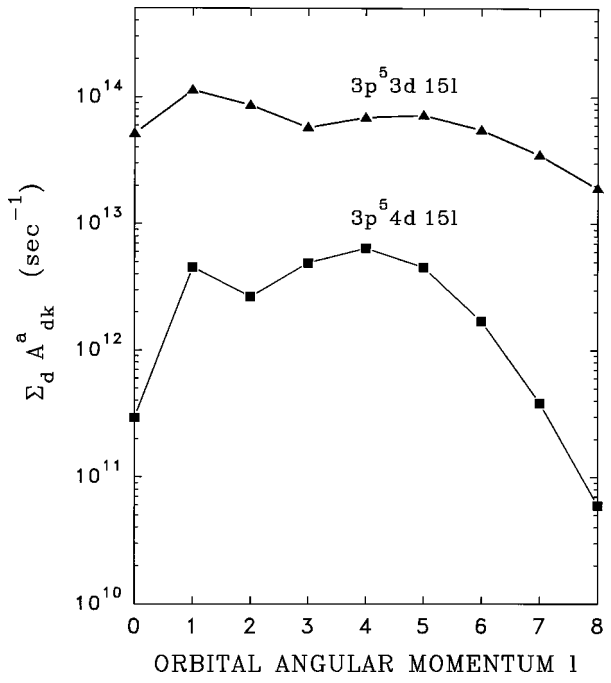

FIG. 2. Sums of the autoionization coefficients $\Sigma_d A^a_{dk}$ to the ground level of the Ar-like ion for the configurations $3p^5 3d 15l$ (triangles) and for $3p^5 4d 15l$ (squares) as a function of the orbital angular momentum quantum number l.

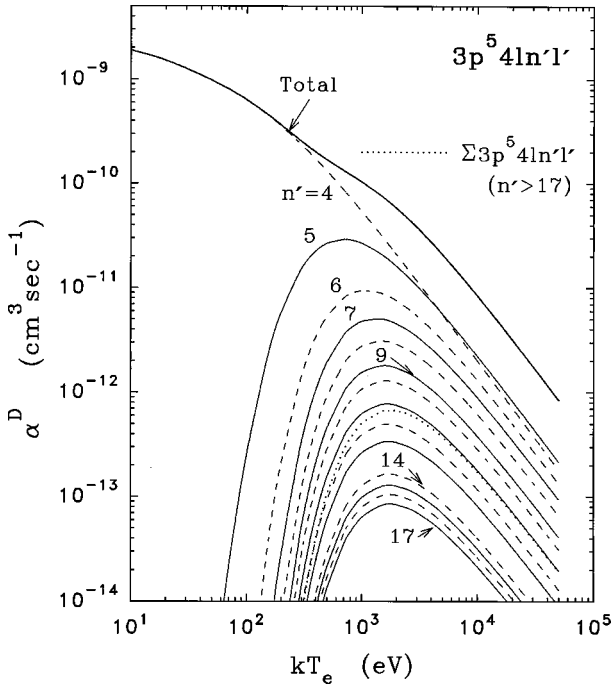

FIG. 3. Partial rate coefficients for DR through the complexes $3p^5 4ln'l'$ ($4 \leqslant n' \leqslant 17$) as a function of the electron temperature. The dotted curve represents the sum of the rate coefficients for all the complexes with $n' > 17$. The thick solid curve is the total rate coefficient for the whole $3p^5 4ln'l'$ complex series.

The DR contributions of the various configuration complexes obtained by level-by-level calculations in the electron temperature range 10 eV $\leqslant kT_e \leqslant$ 50 keV are presented in Fig. 3. At low and medium electron temperature ($kT_e \leqslant$ 5 keV) the dominant contribution comes from the $n' = 4$ complex. This is due to the exponential dependence of the capture rate in Eq. (4) as a function of E_{dk} and to the low E_{dk} values for this complex. In the $n' = 5$ complex all 1299 levels lie above the ionization limit, whereas in the $n' = 4$ complex only 233 out of the 451 levels are above the ionization limit. As a result, at higher electron temperature the contribution of the $n' = 5$ complex becomes larger.

In order to find the value of n_s for this complex series, the DR rate coefficients of the complexes with $4 \leqslant n' \leqslant 17$ are plotted as a function of n' for three different temperatures in Fig. 4. It can be seen that in the range $8 \leqslant n' < 14$ the rate coefficients decrease more steeply than n'^{-3}, whereas for $n' \geqslant 14$ the n'^{-3} behavior takes place as expected. There are two reasons for the fast decrease of the rate coefficients for intermediate n' values. The main reason is the progressive closing of the radiative stabilizing channels to $3p^5 3dn'l'$ [process (c) following Eq. (11)] due to the rising of $3p^5 3dn'l'$ levels above the ionization limit. Finally, for the $3p^5 3d 14l$ complex all the levels are above the ionization limit (as will be shown in Sec. III C) resulting in the sudden steep drop in the $3p^5 4ln'l'$ DR rate coefficients at $n' = 14$. The second reason is the opening of strong autoionization channels to the excited configuration complex $3p^5 4l''$ of the Ar-like ion [process (b) following Eq. (12)]. Thus, a straightforward extrapolation from n' lower than 14 would have led to a significant overestimation of the contributions of the higher complexes.

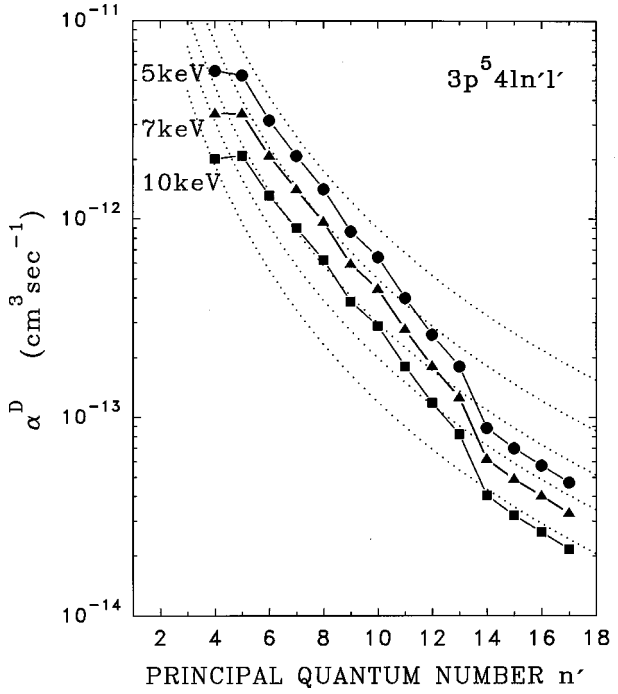

FIG. 4. DR rate coefficients through the complexes $3p^5 4ln'l'$ as a function of the principal quantum number n' in the range $4 \leqslant n' \leqslant 17$ at three different electron temperatures. The solid lines between the calculated values are plotted just to guide the eye. The dotted curves indicate the n'^{-3} grid as a reference for the scaling of the rate coefficients.

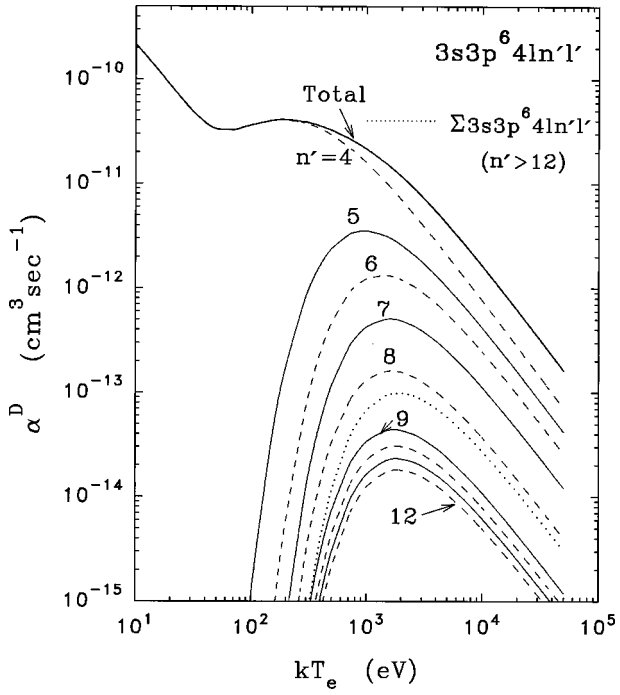

FIG. 5. Partial rate coefficients for DR through the complexes $3s3p^6 4ln'l'$ $(4 \leqslant n' \leqslant 12)$ as a function of the electron temperature. The dotted curve represents the sum of all the rate coefficients for all the complexes with $n' > 12$. The thick solid curve is the total rate coefficient for the whole $3s3p^6 4ln'l'$ complex series.

From the above discussion we conclude that for the $3p^5 4ln'l'$ complex series the usual complex-by-complex extrapolation method [Eq. (9)] can be used, and that n_s should be taken to be 14 or greater. In this study since detailed level-by-level calculations were in fact performed for all the complexes with $4 \leqslant n' \leqslant 17$, n_s was taken to be 17. The sum of the contributions of the complexes with $n' > 18$ evaluated by the complex-by-complex extrapolation method, and the total contribution of all the $3p^5 4ln'l'$ complexes are also shown in Fig. 3. It is clear that for this complex series the relative contribution of high-n' complexes to the total DR rate coefficient is very small.

B. DR through the $3s3p^6 4ln'l'$ complexes

In the $3s3p^6 4ln'l'$ complex series only a few levels of the lower complex $3s3p^6 4l4l'$ are below the ionization limit. All the other complexes are entirely above the ionization limit. The radiative decay processes included in the computations are

$$3s3p^6 4ln'l' \rightarrow 3s^2 3p^6 4l + h\nu, \tag{13}$$

as well as decays to the higher K-like configurations: (a) $3s^2 3p^6 n'l'$, (b) $3s3p^6 3d4l$, (c) $3s3p^6 3dn'l'$ $(n' \leqslant 7)$, (d) $3s^2 3p^5 4ln'l'$ $(n' = 4)$, and (e) $3s3p^6 4ln''l''$ $(n' = 4,\ n'' = 4)$. Again, except for the $3s3p^6 4l4l'$ complex where DAC processes of the forms (d) and (e) are included, the lower levels considered are all below the ionization limit [for this reason $n' \leqslant 7$ in process (c)]. In fact, for the $3s3p^6 4l4l'$ complex the DAC processes are found to be negligible.

The energetically possible autoionization processes included in the calculations are

$$3s3p^6 4ln'l' \rightarrow 3s^2 3p^6 + e^-, \tag{14}$$

as well as autoionization to the higher Ar-like configurations: (a) $3s3p^6 3d$ $(n' \geqslant 5)$, (b) $3s^2 3p^5 4l''$ $(n' \geqslant 7)$, and (c) $3s3p^6 4l''$ $(n' \geqslant 10)$.

As in the case of the $3p^5 4ln'l'$ series, only configurations with $0 \leqslant l' \leqslant 8$ are included in the calculations. In Fig. 5 the DR rate coefficients of the complexes $3s3p^6 4ln'l'$ with $4 \leqslant n' \leqslant 12$ obtained by level-by-level calculations are plotted versus the electron temperature. It can be seen that at all temperatures the dominant contribution comes from the lowest complex $3s3p^6 4l4l'$. It is interesting to note that at electron temperature higher than 1 keV the DR rate coefficient of this complex is as high as one third of the $3p^5 4l4l'$ DR rate coefficient. This is mainly because in the $3s3p^6 4l4l'$ complex almost all the levels lie above the ionization limit, whereas many of the levels belonging to the $3p^5 4l4l'$ complex lie below it. In addition, the $3s3p^6 4l4l'$ complex has no autoionization channels, except for that to the ground level of the Ar-like ion [process (14)].

For the complex series $3s3p^6 4ln'l'$ the behavior of the DR rate coefficient as a function of n' was also checked by the same procedure that was applied for the $3p^5 4ln'l'$ complexes. It was found that in the range $6 \leqslant n' \leqslant 8$ the DR rate coefficient shows a decrease steeper than n'^{-3}, while for $n' \geqslant 9$ the n'^{-3} behavior takes place. The steep decrease of the rate coefficient in the range $6 \leqslant n' \leqslant 8$ is again a consequence of two main reasons: first, the closing of the radiative stabilizing channels [process (c) following Eq. (13)] due to

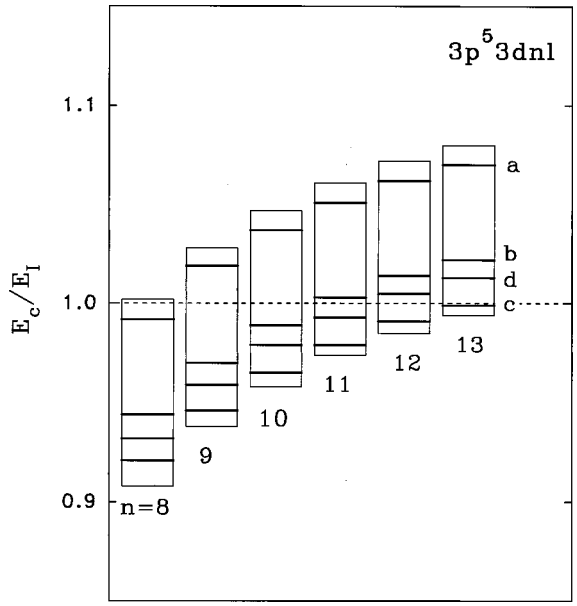

FIG. 6. Energy E_c of the inner-shell excited configuration complexes $3p^5 3dnl$ $8 \leqslant n \leqslant 13$ relative to the first ionization limit E_I. The energies are indicated by a finite vertical range representing the full level spread within each complex. The four thick lines in each complex stand for the mean energy of the four dominant groups of levels (regarding their contributions to the DR rate coefficient). The alphabetic order of the groups is according to the significance of their contributions.

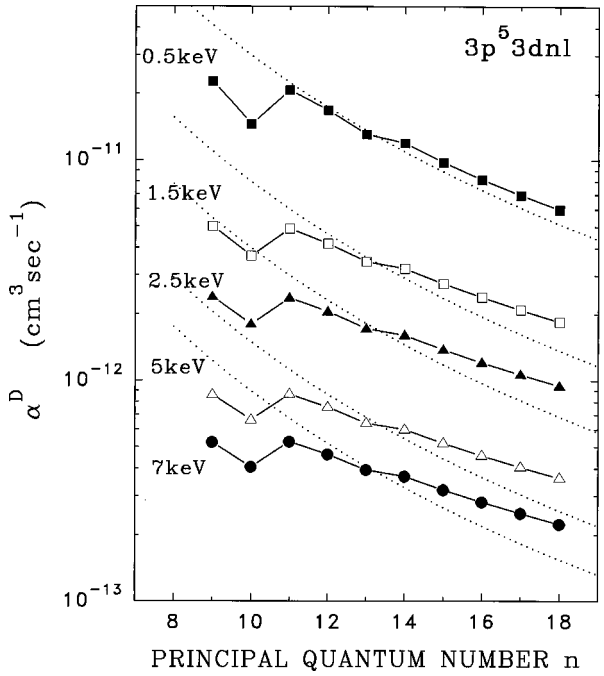

FIG. 7. DR rate coefficients through the complexes $3p^5 3dnl$ as a function of the principal quantum number n in the range $9 \leqslant n \leqslant 18$ at five different electron temperatures. The solid lines between the calculated values are plotted just to guide the eye. The dotted curves indicate the n^{-3} grid as a reference for the scaling of the rate coefficients.

the $3s3p^6 3dn'l'$ levels rising above the ionization limit, and second, the opening of strong autoionization channels [process (b) following Eq. (14)] to the Ar-like excited configurations $3s^2 3p^5 4l''$. Therefore, for the $3s3p^6 4ln'l'$ complex series the usual complex-by-complex extrapolation method [Eq. (9)] can be used starting from $n_s = 9$. Since the detailed level-by-level calculations were already performed up to $n' = 12$ (in order to check the n'^{-3} behavior) n_s is in fact taken to be 12.

The sum of the contributions of the complexes with $n' > 12$ evaluated by the complex-by-complex extrapolation method, and the total contribution of all the $3s3p^6 4ln'l'$ complexes are also shown in Fig. 5. At $kT_e = E_I$, for instance, the total contribution of this complex series to the total DR rate coefficient is found to be 10%.

C. DR through the $3p^5 3dnl$ complexes

The $3p^5 3dnl$ complex series gives the largest contribution to the total DR rate coefficient in the intermediate electron temperature range $100 < kT_e < 1000$ eV. At $kT_e = E_I$ this contribution is about 30% of the total DR rate coefficient.

The special behavior of this complex series is due to the low energy needed for the excitation of the $3d$ electron compared to the ionization energy of the K-like ion in its ground state. As a consequence these complexes start to rise above the ionization limit only when $n \geqslant 8$. Figure 6 shows the energy spread of the $3p^5 3dnl$ complexes near the first ionization limit of the K-like ion. Since n is quite high, level rising with increasing n is very slow. In addition, the energy spread of the complexes is relatively large because of the strong spin-orbit interaction. Consequently, only for $n \geqslant 14$ the $3p^5 3dnl$ complexes lie entirely above the ionization limit.

The processes involved in the dielectronic recombination through these levels were already listed in the beginning of Sec. II. Here these processes are discussed in more detail. The radiative decays considered in the computations are

$$3p^5 3dnl \rightarrow 3p^6 3d + h\nu, \tag{15}$$

as well as decays to the higher K-like configurations: (a) $3p^6 nl$ and (b) $3p^5 3dn'l'$ ($n' \leqslant n$ and $n' \leqslant 13$). For the two lowest autoionizing complexes with $n = 8$ and $n = 9$, DAC processes of the form (b) are also included and are found to have negligible effect. Therefore, for higher complexes DAC processes are neglected.

The energetically possible autoionization processes included for the $3p^5 3dnl$ complexes are

$$3p^5 3dnl \rightarrow 3p^6 + e^- \tag{16a}$$

$$\rightarrow 3p^5 3d + e^- \quad (n \geqslant 10). \tag{16b}$$

In this series also, only autoionizing configurations with $0 \leqslant l \leqslant 8$ are included in the DR calculations. However, here the autoionization coefficients to the ground level of the Ar-like ion decrease relatively slowly with increasing l as shown in Fig. 2 (upper curve). As a result, contributions of higher l-value configurations can be significant as can be seen from Fig. 1. For example, at $kT_e = 1500$ eV the sum of the DR rate coefficients for the $3p^5 3d9l$ configurations with $6 \leqslant l \leqslant 8$ is larger than 25% of the total DR rate coefficient for the whole $3p^5 3d9l$ complex. Thus, detailed level-by-level calculations

and an extrapolation procedure as a function of l may also be needed for the $l>8$ configurations, but this is beyond the scope of the present work.

In Fig. 7 the DR rate coefficients of the complexes $3p^5 3dnl$ with $9 \leqslant n \leqslant 18$ at five different electron temperatures are plotted against n. One can see that in the range $9 \leqslant n \leqslant 14$ there are irregularities in the behavior of the DR rate coefficients, while for $n \geqslant 15$ the decrease is smooth but slower than n^{-3}. The irregularities in the interval $9 \leqslant n \leqslant 14$ results from the rising of more $3p^5 3dnl$ levels above the ionization limit as n increases, and consequently from the opening of new DR channels. In order to explain these irregularities the mean energies of the four dominant groups of inner-shell excited levels are also marked in Fig. 6. For example, the great increase in the DR rate coefficients for $n=11$ is a result of the rising of the second most dominant group (labeled b) above the ionization limit.

The deviation of the rate coefficients from the n^{-3} behavior even for $n>15$ is a consequence of the unique relative magnitudes of the various atomic coefficients involved in the calculation of the DR rate coefficient for each level d: A^a_{dk}, $\Sigma A^a_{dk'}$, ΣA^{la}_{di}, and $\Sigma A^{hi}_{dl'}$ [see Eqs. (4), (6), and (10)]. In this series, especially, the autoionization coefficient A^a_{dk} is high compared to ΣA_{di} for the dominant levels of each complex. In order to illustrate this effect let us consider the extreme case in which $A^a_{dk} \gg \Sigma A^{lo}_{di}$. For simplicity we assume also that $\Sigma A^{hi}_{di'}=0$ and that $\Sigma A^a_{dk'}=A^a_{dk}$. In this case, the branching ratio in Eq. (6) becomes

$$B^D(d) \approx \frac{\sum_i A^{lo}_{di}}{A^a_{dk}}. \tag{17}$$

Since A^a_{dk} appears also in expression (4) for the dielectronic capture rate, it cancels, and the DR rate coefficient of the level d depends only on ΣA^{lo}_{di}. Now, ΣA^{lo}_{di}, which is the sum of the Einstein coefficients for spontaneous radiative decays that involve only the $3d$ excited electron, is independent of n. Thus, in this simple example the DR rate coefficient for the level d will be approximately independent of n until n is large enough so that $A^a_{dk} < \Sigma A^{lo}_{di}$. Only then, for very high n values, the DR rate coefficient of the level d will decrease steeply as n^{-3}.

When the atomic coefficients of the levels pertaining to the $3p^5 3dnl$ complexes for n values around 15 were examined, it was found that for the most dominant levels in each configuration $A^a_{dk} > \Sigma A^{lo}_{di}$. In some cases A^a_{dk} was larger than ΣA^{lo}_{di} by a factor of 2 and in other cases it was even an order of magnitude larger. Keeping this in mind, it is not surprising that for the $3p^5 3dnl$ complexes the rate coefficients decrease slower than n^{-3}. The result is that contrary to the other series, here one cannot apply the simple complex-by-complex extrapolation method [Eq. (9)], and the more detailed level-by-level extrapolation procedure [Eq. (10)] must be used. Actually, in this work detailed level-by-level calculations were performed, for $8 \leqslant n \leqslant 18$, and n_s in Eq. (10) was taken to be 18.

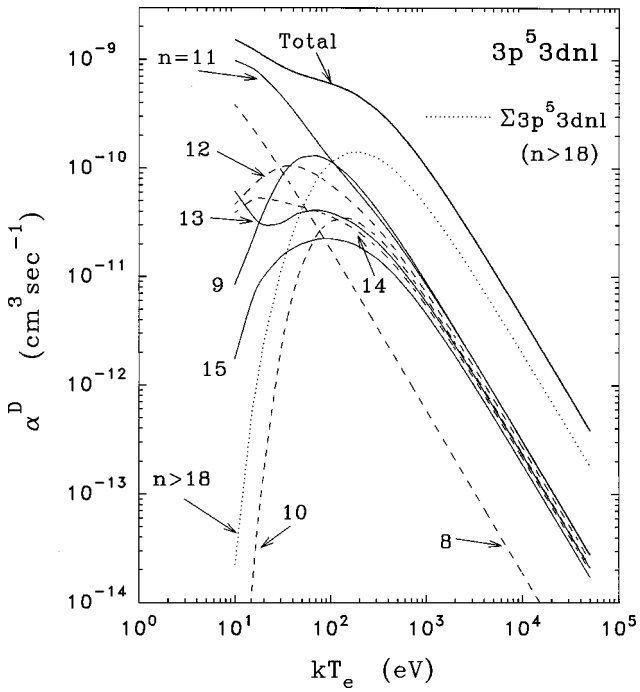

FIG. 8. Partial rate coefficients for DR through the complexes $3p^5 3dnl$ ($8 \leqslant n \leqslant 18$) as a function of the electron temperature. The dotted curve represents the sum of the rate coefficients for all the complexes with $n>18$. The thick solid curve is the total rate coefficient for the whole $3p^5 3dnl$ complex series.

Figure 8 shows the DR contributions of the complexes $3p^5 3dnl$ with $8 \leqslant n \leqslant 15$ obtained by detailed calculations as a function of the electron temperature in the range $10\ \text{eV} \leqslant kT_e \leqslant 50\ \text{keV}$. One can see the irregularities in the behavior of the rate coefficients as n increases. As discussed above these irregularities result from the rising of inner-shell excited levels above the ionization limit as n increases (see Fig. 6) leading to the opening of new DR channels. This is especially pronounced at low electron temperatures. At these temperatures inner-shell excited autoionizing levels lying close to the first ionization limit can give a significant contribution to the total DR rate coefficient. Indeed, the maximum value of the DR rate coefficient for a given level d as a function of T_e is reached at $kT_e = 2/3 E_{dk}$ and is proportional to $(E_{dk})^{-3/2}$. Therefore, if E_{dk} is sufficiently small the DR contribution of this level can be very important at low electron temperatures. (For a more detailed discussion see Ref. [5].)

The sum of the contributions of the complexes with $n>18$, deduced from the level-by-level extrapolation procedure, and the total contribution of all the $3p^5 3dnl$ complexes are also shown in Fig. 8. In contrast to the previous cases, for this complex series the contributions of the high-n complexes is very significant. These contributions were neglected in the DR calculations for Ar-like molybdenum (Ref. [7]). Here, for W^{56+}, the contribution of the $n>18$ complexes is more than 40% of the total DR rate coefficient of the whole $3p^5 3dnl$ series at an electron temperature higher than 500 eV. It should be noticed that using the ordinary complex-by-complex extrapolation procedure for the high

$3p^5 3dnl$ complexes might lead to a significant underestimation of the DR rate coefficient.

D. DR through the $3s3p^6 3dnl$ complexes

In the $3s3p^6 3dnl$ complex series the $n=7$ complex is the first complex in which there are levels above the ionization limit. For $n \geqslant 8$ all the levels in each complex lie above the first ionization limit. The radiative decays included in the computations are

$$3s3p^6 3dnl \rightarrow 3s^2 3p^6 3d + h\nu, \tag{18}$$

as well as decays to the higher K-like configurations: (a) $3s^2 3p^5 3dnl$ ($n \leqslant 13$) and (b) $3s3p^6 3dn'l'$ ($n' \leqslant 8$). Except for the $n=7$ and $n=8$ complexes where DAC processes of the forms (a) and (b) are included, the lower levels considered are all below the ionization limit. For $n=7$ the effect of the DAC processes is found to be negligible. For $n=8$ the DAC processes decrease the rate coefficient by 5% at electron temperatures higher than 800 eV.

The energetically possible autoionization processes taken into account are

$$3s3p^6 3dnl \rightarrow 3p^6 + e^- \tag{19a}$$

$$\rightarrow 3p^5 3d + e^- \quad (n \geqslant 8). \tag{19b}$$

Autoionization processes to the Ar-like excited configuration $3s3p^6 3d$ were found to be energetically forbidden for $n \leqslant 18$ (at least) and thus were not taken into account.

Autoionizing inner-shell excited configurations with $0 \leqslant l \leqslant 8$ are included in the calculations. Here this is fairly well justified by the fact that already for $n \geqslant 14$ the radiative stabilization channel [process (a) following Eq. (18)] is closed (see Sec. III C). Therefore, neglecting DAC processes, the remaining radiative decays are via processes of the forms (18) and (b) following (18). Since n' is limited to 7 (and $l' \leqslant 6$), there are no stabilization channels for levels with $l > 7$. Under the above assumption the DR rate coefficients of these levels are simply zero.

In Fig. 9 the DR rate coefficients computed by detailed calculations for the complexes $3s3p^6 3dnl$ with $7 \leqslant n \leqslant 18$ are given as a function of the electron temperature. At low electron temperatures ($kT_e < 700$ eV) the dominant DR contribution comes from the $3s3p^6 3d7l$ complex due to the low E_{dk} values of the levels belonging to this complex. At higher electron temperatures the contribution of the $3s3p^6 3d8l$ complex is dominant since for this complex all the levels are above the first ionization limit. One notices the great decrease of the DR rate coefficient for $3s3p^6 3d9l$. As in the cases of $3s3p^6 4ln'l'$ and $3p^5 4ln'l'$, this is due to opening of strong autoionization channels (in this case to the $3p^5 3d$ excited configuration of the Ar-like ion), and to the closing of some important radiative stabilization channels [of the form (a) following (18)].

The behavior of the DR rate coefficients as a function of n was checked in this series too. It was found that in the range $8 \leqslant n \leqslant 14$ there are abrupt drops arising from the opening of strong autoionization channels of the form (19b), and also from the closing of important radiative stabilization channels

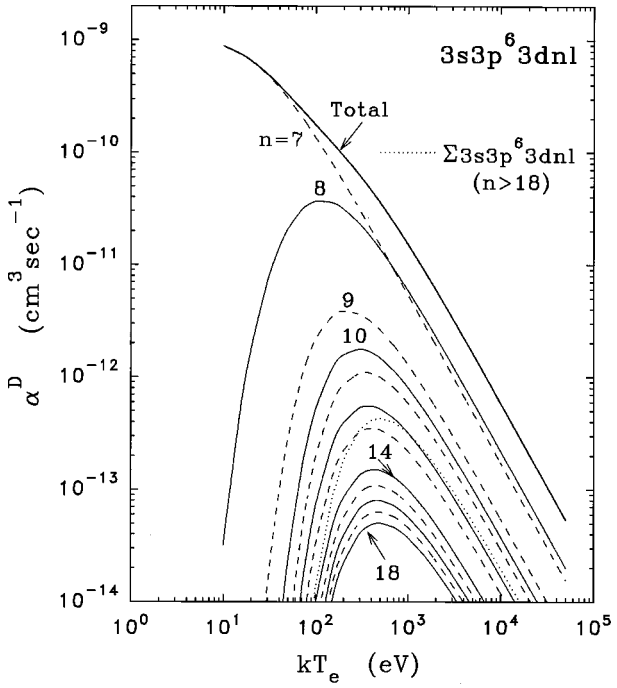

FIG. 9. Partial rate coefficients for DR through the complexes $3s3p^6 3dnl$ ($7 \leqslant n \leqslant 18$) as a function of the electron temperature. The dotted curve represents the sum of the rate coefficients for all the complexes with $n > 18$. The thick solid curve is the total rate coefficient for the whole $3s3p^6 3dnl$ complex series.

of the form of (a) following Eq. (18), due to the rising of the lower $3s^2 3p^5 3dnl$ levels above the first ionization limit. Only for $n \geqslant 15$ does the n^{-3} behavior take place. Hence for this complex series, the usual complex-by-complex extrapolation method [Eq. (9)] can be used starting from $n_s = 15$. Since detailed level-by-level calculations were already performed up to $n=18$, n_s was taken to be 18. One notices that a naive approach of taking n_s to be 8 would have led to a significant overestimation of the contributions of the higher complexes.

Figure 9 also shows the sum of the contributions of the complexes with $n > 18$ obtained by complex-by-complex extrapolation and the total contribution of all the $3s3p^6 3dnl$ complexes. At $kT_e = E_I$, for instance, this complex series is found to contribute about 4% to the total DR rate coefficient.

E. DR through the $2p^5 3s^2 3p^6 3dnl$ complexes

Since in the $2p^5 3s^2 3p^6 3dnl$ complex series an electron from the inner shell L is excited, all the complexes ($n \geqslant 3$) lie high above the first ionization limit. As a result, there are many possible autoionization channels. Also, their contributions to the total DR rate coefficient becomes significant only at very high electron temperature.

The radiative transitions considered for this complex series are

$$2p^5 3s^2 3p^6 3dnl \rightarrow 2p^6 3s^2 3p^6 3d + h\nu, \tag{20}$$

as well as decays to the higher K-like configurations: (a) $2p^6 3s^2 3p^6 nl$ and (b) $2p^6 3s3p^6 3dnl$ ($n \leqslant 7$). In all these

transitions the lower levels considered are below the first ionization limit [$n \leqslant 7$ in process (b)]. For $n=4$ we also consider DAC processes of the form

$$2p^5 3s^2 3p^6 3d4l \rightarrow 2p^5 3s^2 3p^6 3dn'l' + h\nu \quad (n'=3,4). \tag{20'}$$

However, the DAC processes are found to have negligible effect on the DR rate coefficients.

The energetically possible autoionization processes involving the high orbital nl electron taken into account are

$$2p^5 3s^2 3p^6 3dnl \rightarrow 2p^6 3s^2 3p^6 + e^-, \tag{21}$$

as well as autoionization to the higher Ar-like configurations: (a) $2p^6 3s^2 3p^5 3d$, (b) $2p^6 3s 3p^6 3d$, and (c) $2p^5 3s^2 3p^6 3d$ ($n \geqslant 6$). In addition, we include the autoionization processes which do not involve the nl electron, to the Ar-like configurations: (d) $2p^6 3s^2 3p^5 nl$, (e) $2p^6 3s^2 3p^4 3dnl$, (f) $2p^6 3s 3p^6 nl$, (g) $2p^6 3s 3p^5 3dnl$, and (h) $2p^6 3p^6 3dnl$. Processes (d)–(h), which have atomic coefficients independent of n, and are found to be the dominant autoionization channels in this complex series, were neglected in previous DR calculations for Ar-like molybdenum (Ref. [7]). As in the case of the $3p^5 4ln'l'$ series, configurations with high l values have negligible contributions. Thus, only configurations with $0 \leqslant l \leqslant 8$ are included in the calculations.

Detailed calculations of the DR rate coefficients of the complexes $2p^5 3s^2 3p^6 3dnl$ were performed for $3 \leqslant n \leqslant 8$. The results show that the dominant DR contribution at all temperatures comes from the $2p^5 3s^2 3p^6 3d^2$ configuration.

Upon checking the behavior of the DR rate coefficients as a function of n, one finds that the expected n^{-3} scaling takes place already from $n=4$ without irregularities. This is in spite of the closing of stabilizing radiative channels [process (b) following Eq. (20)] and the opening of autoionization channels [process (c) following Eq. (21)]. In fact, these channels are not the dominant channels in this series and thus, do not affect the scaling of the DR rate coefficients as a function of n. As a result, Eq. (9) for the ordinary complex-by-complex extrapolation method can be used with $n_s=4$. Since detailed level-by-level computations were performed up to $n=8$, n_s was actually taken to be 8. The sum of the DR contributions of all the complexes with $n>8$ obtained by extrapolation reaches about 10% of the total contribution of the $2p^5 3s^2 3p^6 3dnl$ complex series at high temperature ($kT_e > 2$ keV). Finally, all this complex series contributes about 6% of the total DR rate coefficient at $kT_e = E_I$ and more than 10% for $kT_e \geqslant 10$ keV.

F. DR through the $2s2p^6 3s^2 3p^6 3dnl$ complexes

The $2s2p^6 3s^2 3p^6 3dnl$ complex series lie even higher than the $2p^5 3s^2 3p^6 3dnl$ series. All the complexes are entirely above the first ionization limit and include fewer levels per complex. Moreover, the radiative stabilization channels are comparatively weaker than those of the $2p^5 3s^2 3p^6 3dnl$ complexes. Therefore, the contribution of these complexes to the total DR rate coefficient is expected to be small.

The radiative transitions included in the computations are

$$2s2p^6 3s^2 3p^6 3dnl \rightarrow 2s^2 2p^6 3s^2 3p^6 3d + h\nu \tag{22a}$$

$$\rightarrow 2s^2 2p^6 3s^2 3p^5 3dnl + h\nu. \tag{22b}$$

Autoionization processes to the same Ar-like excited configuration complexes that were included for the $2p^5 3s^2 3p^6 3dnl$ complexes [see Eq. (21) and processes (a)–(h) following Eq. (21)] are possible and are included in the present calculations.

Since the contribution of this complex series is quite small and since for high complexes the dominant radiative stabilizing channels (22b) are gradually closed (neglecting DAC) the detailed level-by-level calculations are performed only in the range $3 \leqslant n \leqslant 5$ and no extrapolation is made. We estimate the error introduced by not including the higher complexes to be less than 1% of the total rate coefficient at all electron temperatures. The results of the calculations show that for $kT_e = E_I$ this complex series contributes only 0.6% of the total DR rate coefficient. At very high electron temperatures ($kT_e = 50$ keV) the contribution is still less than 2%.

G. DR through the $3p^5 5l5l'$ complex

Finally, the contribution of the configuration complex $3p^5 5l5l'$ is considered. The radiative decay processes taken into account in the computations are

$$3p^5 5l5l' \rightarrow 3p^6 5l' + h\nu \tag{23a}$$

$$\rightarrow 3p^5 3d5l' + h\nu. \tag{23b}$$

In this case no DAC processes were included. The energetically possible autoionization processes considered are

$$3p^5 5l5l' \rightarrow 3p^6 + e^- \tag{24}$$

as well as autoionization to the higher Ar-like configurations: (a) $3p^5 3d$ and (b) $3p^5 4l''$. The results of the calculations show that this complex contributes about 2% of the total DR rate coefficient at electron temperatures higher than E_I. Since the contribution of this complex is relatively small and since for higher complexes belonging to the $3p^5 5ln'l'$ series a part of the important radiative channels are closed and new autoionization channels are opened, the contributions of the higher complexes ($n' > 5$) are disregarded here. The underestimation caused by this approximation is negligible at low electron temperature and is estimated to be about 3% of the total DR rate coefficient at high temperature.

H. Total DR rate coefficient

The total DR rate coefficient, obtained by adding the DR contributions of all the complex series discussed in the previous sections, is given as a function of the electron temperature in Fig. 10 and in Table I. For comparison, Fig. 10 also shows the total contribution of each series. These results show that the largest contribution at low electron temperatures ($kT_e < 100$ eV) and at high electron temperatures ($kT_e > 1$ keV) comes from the complex series $3p^5 4ln'l'$, while in the intermediate range $100 < kT_e < 1000$ eV the $3p^5 3dnl$ complexes give the largest contribution. The im-

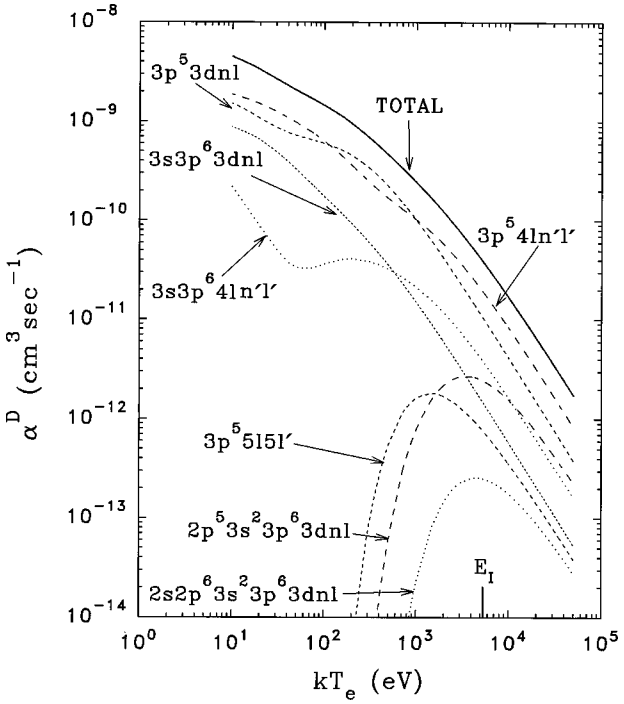

FIG. 10. The total DR rate coefficient for Ar-like W (thick curve) and the total contributions of the various complex series included in this work as a function of electron temperature. E_I is the first ionization energy of the K-like ion.

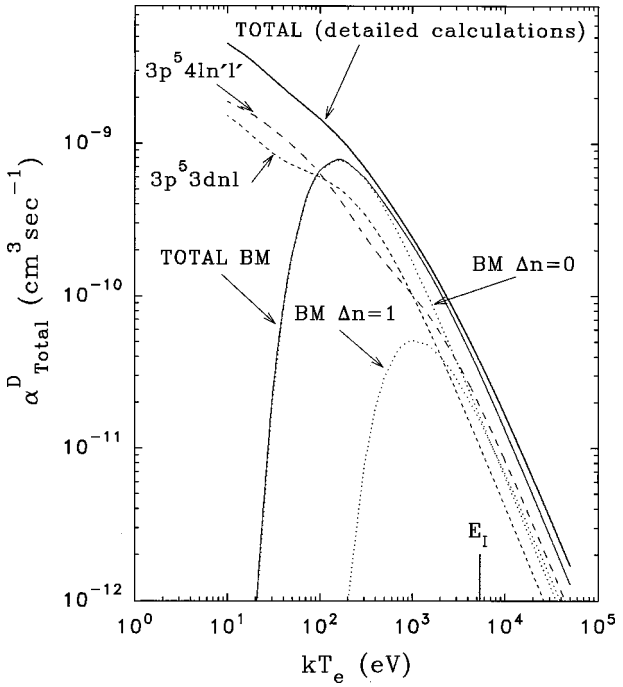

FIG. 11. Comparison of the detailed level-by-level calculations (thick solid curve) and the BM approximation (solid curve) for the total DR rate coefficient of Ar-like W. The long dashed curve is the total rate coefficient for the $3p^5 4ln'l'$ complex series. The short dashed curve is the total rate coefficient for the $3p^5 3dnl$ complex series. The two dotted curves are the corresponding BM results for these two series ($\Delta n=1$ for $3p^5 4ln'l'$ and $\Delta n=0$ for $3p^5 3dnl$). E_I is the first ionization energy of the K-like ion.

portance of the $3p^5 4ln'l'$ DR contribution is a consequence of the large Einstein coefficients for the $3l$-$4l'$,$\Delta n=1$ radiative transitions. These coefficients scale approximately like r^4 where r is the charge of the ion core ($r=56$ in the present work). In contrast, the $3p$-$3d$,$\Delta n=0$ transitions, which are important in the stabilization of the $3p^5 3dnl$ complexes, scale only linearly with r and are much smaller here. Nevertheless, the DR contribution of the whole $3p^5 3dnl$ series is very important in the intermediate electron temperature range due to the large cumulative contribution of a great number of high-n complexes that lie very close to each other in energy (see Fig. 8). One should notice that for light elements of the Ar I isoelectronic sequence the $3p^5 3dnl$ DR contribution is expected to be dominant at all temperatures because of the different dependence of the radiative rates upon r. In fact, it was shown by Fournier *et al.* [7] that this is indeed the case for Mo^{24+}.

TABLE I. Total DR rate coefficient (in cm^3 sec^{-1}) for Ar-like tungsten as a function of the electron temperature kT_e (in eV). $X[-Y]$ denotes $X\times 10^{-Y}$.

kT_e (eV)	Total DR rate coefficient (cm^3 sec^{-1})
10	4.50[−09]
20	3.32[−09]
30	2.68[−09]
50	2.06[−09]
100	1.45[−09]
200	9.51[−10]
300	7.03[−10]
500	4.59[−10]
1000	2.45[−10]
2000	1.21[−10]
3000	7.72[−11]
5000	4.18[−11]
7000	2.72[−11]
10000	1.70[−11]
20000	6.52[−12]
30000	3.65[−12]
50000	1.74[−12]

In Fig. 11 the total DR rate coefficient calculated in the present work is compared to the results obtained from the semiempirical Burgess-Merts (BM) approximation [15,16]. The BM results shown in the figure were obtained using the oscillator strengths and the transition energies computed by RELAC [12] for the $3p$-$3d$ ($\Delta n=0$) and the $3p$-$4d$ ($\Delta n=1$) transitions only, as suggested by Breton *et al.* [17]. It can be seen that at low electron temperature ($kT_e<100$ eV) the BM approximation greatly underestimates the DR rate coefficient. The explanation for this discrepancy is thoroughly discussed in Ref. [6]. At higher electron temperatures, however, there is quite a good agreement between the BM approximation and the detailed level-by-level calculations. For example, at $kT_e=E_I$, the BM approximation underestimates the total rate coefficient by only 15%. At very high electron temperature ($kT_e\simeq 50$ keV) the BM approximation underestimates the total rate coefficient by about 25%. It should be stressed that the relatively good agreement for the total DR rate coefficient for $kT_e>100$ eV may be somewhat fortuitous here; indeed, a noticeable discrepancy is observed for the

individual contribution of each of the complex series considered. For instance at $kT_e = E_I$, the $\Delta n = 1$ BM approximation value is 20% *lower* than the calculated DR rate coefficient for the $3p^5 4ln'l'$ series, whereas the $\Delta n = 0$ BM value is 55% *higher* than the $3p^5 3dnl$ series DR rate coefficient. Thus, for other elements in the Ar I isoelectronic sequence the deviation of the BM approximation from the calculated total DR rate coefficient can be significantly larger as is found in the Ni I sequence [6].

IV. CONCLUSIONS

Extensive level-by-level calculations of the DR rate coefficient for Ar-like W^{56+} ion in the ground state were performed. The results show that the two complex series $3p^5 4ln'l'$ and $3p^5 3dn'l'$ give the most important contribution ($\simeq 75\%$) to the total DR rate coefficient. The largest contribution in the relevant electron temperature range ($kT_e \simeq E_I$) comes from the complex series $3p^5 4ln'l'$. This is due to the large Einstein coefficients for the $3l$-$4l'$, $\Delta n = 1$ radiative transitions involved in the DR recombination process through levels belonging to this series. However, other complex series such as $3s3p^6 4ln'l'$, $3s3p^6 3dn'l'$, and $2p^5 3s^2 3p^6 3dn'l'$ were found to give contributions that cannot be disregarded.

The n' dependence of the DR rate coefficients in each complex series was checked. In most cases it was found that for low-n' values there are irregularities. These irregularities are due to the opening of new DR channels, to the closing of radiative stabilization channels, and to the opening of new autoionization channels. For higher n' values the expected n'^{-3} behavior along a series takes place in all cases except for the $3p^5 3dn'l'$ series. Therefore, for all complex series except for the $3p^5 3dn'l'$ series the usual complex-by-complex extrapolation procedure is used in order to evaluate the DR contributions of the high-n' complexes. In the $3p^5 3dn'l'$ series, the Einstein coefficients (ΣA_{di}) are smaller than the autoionization coefficients (A^a_{dk}) for the dominant levels. As a result, the DR rate coefficients decrease slower than n'^{-3} and the more detailed level-by-level extrapolation method is applied. Moreover, because of the slow decrease of the DR rate coefficients with increasing n', in this latter case the contributions of very-high-n' complexes is important and the question of density effects arises.

In addition to the n' dependence, the l' dependence was also checked for the various complex series. It was found for the $3p^5 3dn'l'$ complexes that high-l' values contribute significantly; in all other cases the contributions of high-l' values are negligible. Thus, for the $3p^5 3dn'l'$ complexes it is desirable to find an approximate extrapolation procedure for evaluating the high-l' contributions.

A comparison of the Burgess-Merts approximation with the results of the present detailed level-by-level calculations shows that the former greatly underestimates the total DR rate coefficient at low electron temperatures ($kT_e < 100$ eV). However, in the electron temperature range $kT_e \simeq E_I$ the underestimation is only 15% of the total DR rate coefficient. This fairly good agreement may be fortuitous here; for other elements in the Ar I sequence the deviation is expected to be larger as is found in the Ni I sequence. Hence, further detailed level-by-level calculations are required for the other elements in the Ar I isoelectronic sequence.

ACKNOWLEDGMENTS

We are thankful for fruitful discussions with R. Doron and D. Mitnik, and their valuable comments. We also wish to thank A. Bar-Shalom of the Ben-Gurion University of Beer-Sheva, Israel, M. Klapisch of the Naval Research Laboratory, and W. H. Goldstein of the Lawrence Livermore National Laboratory for the use of the HULLAC code package. One of the authors (E.B.) was supported by the Charles Clore Israel Foundation.

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